Final Technical Status Report

on

Investigation of Contact Failures on Resistors

NASA Contract No. NAS5-9322

19 October 1966

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SUMMARY

An investigation was conducted to determine and eliminate the incidence of defective electrical contacts of aluminum interconnecting films to poly-crystalline silicon resistors. A solution was found during the contract period. The solution was determined by combining critical geometry design with an improved alloy cycle. In general, the geometrical perturbation was the most significant factor in producing good electrical contact of the aluminum films to the silicon resistors.

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Section 1
INTRODUCTION

1.1 PURPOSE

The purpose of this program was to determine the cause of defective electrical contacts observed to be good immediately prior to contact alloying, but defective immediately subsequent to alloying. The failure produced an open circuit between the aluminum interconnecting film and the silicon resistor. Upon determination of the failure mechanism, effort was directed toward elimination of the failures.

1.2 STATEMENT OF WORK

The investigation provided information in three separate areas:

- failure mechanisms
- formulation of solutions
- empirical investigation to prove above theories.

Since the work was necessitated by the open-circuit failure, a test vehicle was designed to provide the information required to solve the failure. The test vehicle was used primarily to reproduce the observed failure by perturbations in the alloy cycle. It was felt that better factual information could be extrapolated from the accumlator blocks themselves.

Section 2
DISCUSSION

2.1 PRIMARY CONSIDERATIONS

It was found that the use of the original geometrical contact design and cycling through the standard contact alloy propagated what initially appeared to be an excessive solid solubility of poly-crystalline silicon into aluminum beyond the maximum solubility limitation. However, it is suggested that a quasi-surface phenomenon, rather than an excessive solubility mechanism, was the cause for the observed failure.

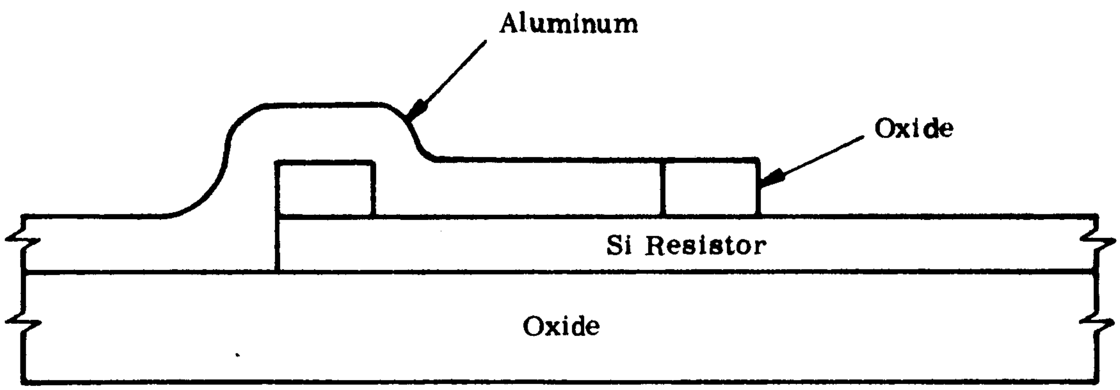
It should be noted that it would be highly improbable that either basic bulk properties prevailed or that ideal phase equilibria existed during the alloy cycle. The actual characteristics of the thin films involved are not fully understood at this time.

2.2 FAILURE MODES

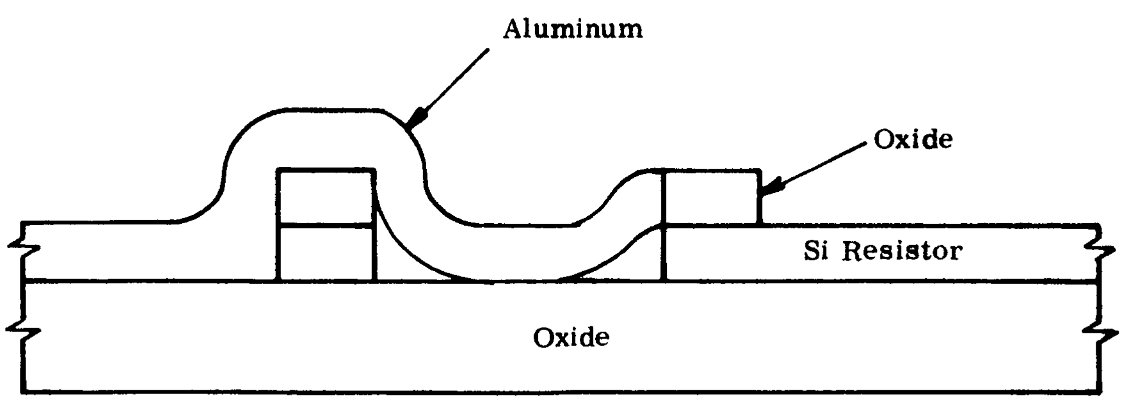
A detailed investigation was conducted to determine the mechanism of failure. Theoretical mechanisms were proposed and experiments were conducted to satisfy the postulates. As previously mentioned, most of this work was conducted on the test vehicle and information was obtained with respect to alloy cycle perturbation and geometry of contact.

2.2.1 Existing Failure Mode

Basically, the failure may be categorized as a total transport of the silicon away from the contact area. This removal of silicon would result in an open in the resistor circuit. Figure 1 is a schematic representation of the failure mechanism.



(a) Configuration Prior to Alloy



(b) Observed Cause of Open Circuitry

Fig. 1 Schematic Representation of the Failure Mechanism

From Fig. 1, there are two possible mechanisms which could be responsible for the failure — either an increased solid solubility concentration of available silicon into the aluminum film, or a reduction in "surface" energies, permitting migration to occur. In either case, it should be assumed that there is a limitation on the amount of available silicon.

Although a total removal of silicon was observed in certain cases, there was the possibility of aluminum contacting the ends of the resistors. However, this contact was not sufficient to produce good ohmic contact, and undoubtedly an open resistor circuit would result.

2.2.2 Excessive Solubility

Examination of the Si-Al binary eutectic phase equilibrium diagram reveals that the maximum theoretical solid solubility content of silicon into aluminum is 1.59 weight %. From the examination of Fig. 2, and considering the total amount of silicon and aluminum available, it would be impossible to reduce the silicon sufficiently to cause an electrical open circuit. Since a maximum of 1.59 weight % may go into solution during an alloy cycle, after the entire reaction has occurred there should be sufficient silicon remaining at the contact area to yield a completed circuit.

2.2.2.1 Increased Solubility. With reference to Fig. 2, there exists one method of increasing the solubility of silicon into aluminum, thereby totally depleting the contact area of silicon. This method requires that the alloying be performed at a temperature above the eutectic isotherm. This type of alloying would produce the eutectic composition of Si-Al and allow complete depletion of silicon from the contact area. However, all contact alloying was performed sufficiently below the eutectic isotherm to eliminate this possibility.

2.2.2.2 Alkali Ions. It has been reported[1] that an addition of alkali ions to the Si-Al system may reduce the eutectic temperature. The extent of the eutectic

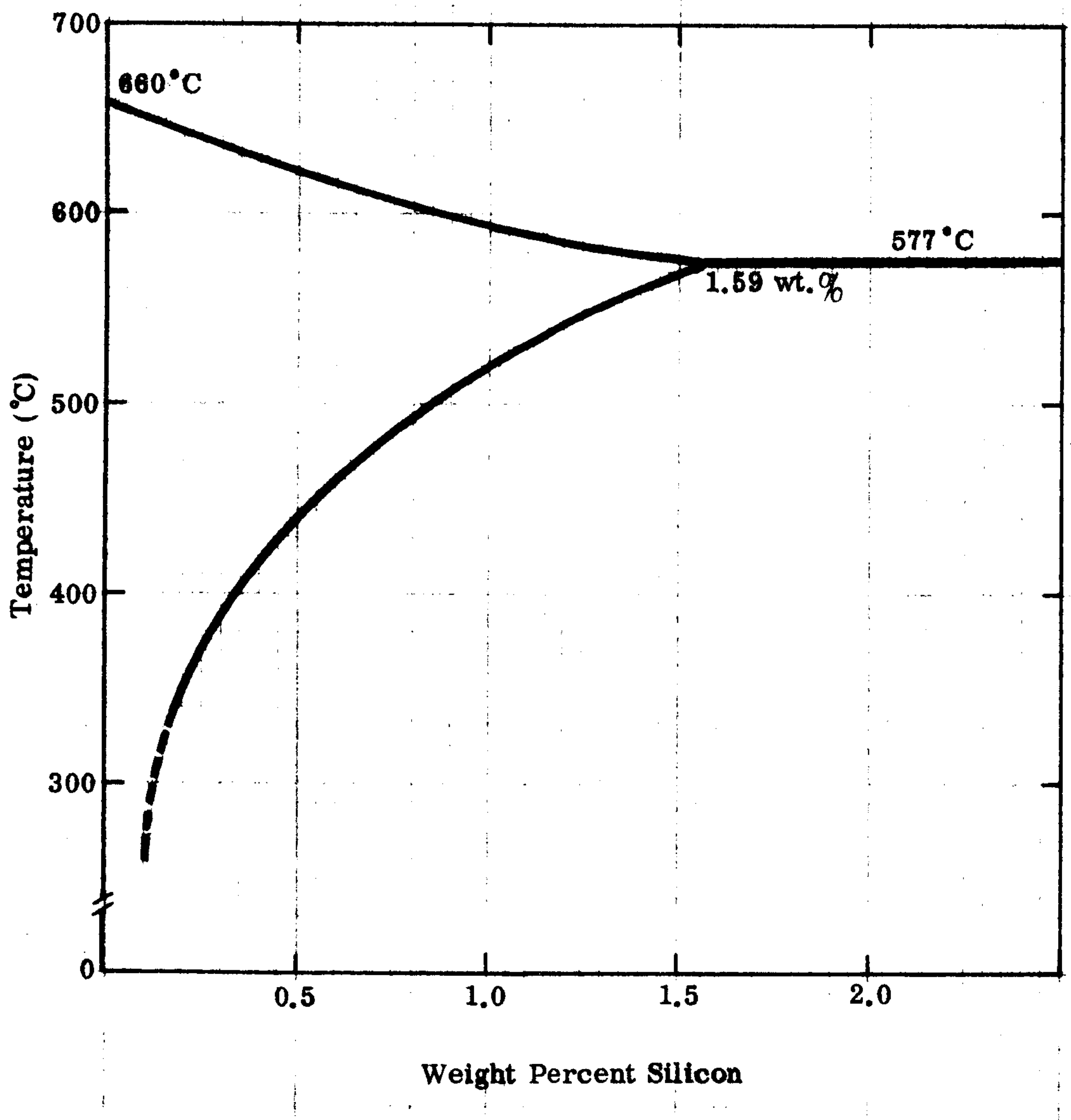


Fig. 2 Partial Phase Equilibrium Diagram of Si-Al System After Hansen

reduction depends upon the conditions of modification. This method of increased solubility also seems unlikely since the presence of alkali ions in MOS devices degrades the stability characteristics. The degradation of device stability has not been a problem associated with the MOS devices fabricated into the resistor circuit. Therefore, it is improbable that there was an increase in the solubility of silicon into aluminum by a eutectic isotherm shift.

2.2.2.3 Localized Heating. Localized heating also may contribute to the increased solubility by raising certain areas beyond the eutectic temperature. However, this reaction would be infrequent and could not account for the total removal of silicon from the contact area.

2.2.2.4 Hume-Rothery Considerations. Assuming that the rule of non-reciprocity holds[2], according to the Hume-Rothery considerations for alloy formation, the tetravalent silicon should dissolve to a greater extent in the trivalent aluminum than in the reverse case. This has been observed to hold, and if a total extrapolation of the rule is assumed, the possibility of increasing the solubility of silicon in aluminum exists at an elevated temperature, if held at that temperature for a sufficient time. This would then be a diffusion-controlled reaction and actual solubility would remain constant, although depletion of silicon might occur.

2.2.3 Phase Diagram Considerations

It should be realized that the above postulations reflect on the ideal case of aluminum in contact with poly-crystalline silicon. The ideal case does not exist for a simple binary reaction since both boron and oxygen are present. To effectively evaluate the failure mechanism, a quaternary phase equilibrium diagram should be consulted. However, this also would be inadequate since the initial assumption was that equibrium during the alloy cycle does not exist.

2.2.4 Surface Mechanisms

With the assumption that phase equilibrium does not exist, the only remaining solution to the failure mechanism would be a diffusion reaction. Although basic bulk properties are not entirely followed, crystallographic orientations are present. The small grains present in the poly-crystalline silicon could diffuse rapidly along the grain boundaries of the aluminum. During the alloy cycle, it appears that this mechanism is dominant. However, on an atomic scale the complete reaction would be a two-phase reaction. Initially a small amount of silicon would reach the maximum solubility content, and this would be followed by the depletion of the contact area by a diffusion mechanism. This dual-stepped reaction would account for the volume-to-area ratio. The aluminum volume available would be sufficient to deplete the silicon area at the contact points if the diffusion mechanism was dominant. Since there is a lowering of the surface energy, due to the elevated temperature of alloy, and since the gradient of distribution is temperature-dependent, it is very possible that the diffusion reaction could exist.

Observed Migration. During the investigation, it was found that the reaction causing the open circuit occurred at a higher rate in the regions connected to a "heat sink," i.e., a probe pad. This preferential reaction was observed during the investigation and is shown schematically in Fig. 3.

The total migratory travel of the silicon is determined by the time and temperature of the alloy cycle. Aluminum possesses a very high rate of diffusion into silicon[3]. The reverse case also should be assumed to hold true. Since the poly-crystalline silicon was evaporated, a loose packing structure would be expected. Therefore, this type of structure would be loosely bonded, allowing the kinetic reaction to proceed at a relatively low activation energy. Since the activation energy is temperature-dependent, it is sufficient to say that diffusion of the type described above would be possible. Also, the reaction observed where the silicon is preferentially dissolved could be explained according to the

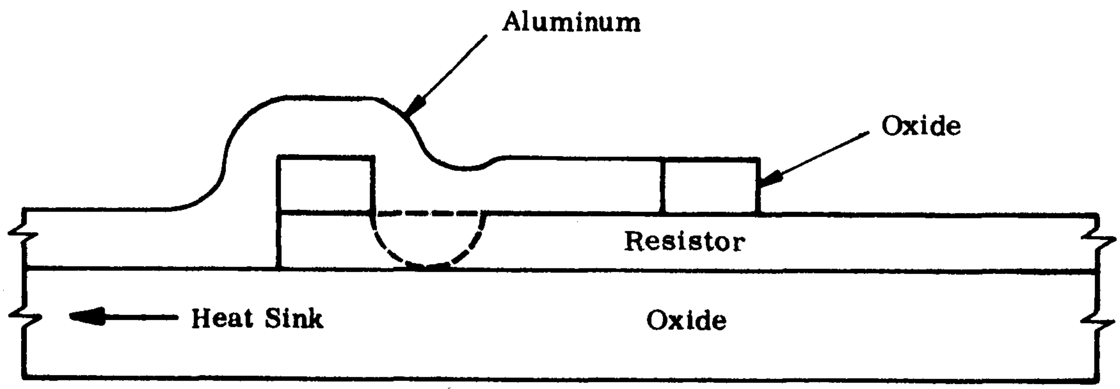


Fig. 3 Preferential Dissolution of Si into Al During Alloy

excess heat maintained on the side of a large heat reservoir, permitting a faster diffusion in that particular area.

2.2.5 Failure Mode Considerations

In the final analysis two important interdependent film characteristics should be considered. First, the films of silicon are loosely packed; and secondly, the mechanism of film dissolution is controlled by a diffusion process.

2.2.5.1 Silicon Films. Although it was suggested in Section 2.2.2 that sufficient silicon was present for maximum solid solubility, due to the loosely packed array of the silicon, the volume ratio appears to be an important factor in determining dissolution. If an infinite volume of aluminum exists, the loosely packed array of poly-crystalline silicon would not be limited to solubility at the interface. The entire volume of silicon would tend to saturate the aluminum to its maximum solubility content, thereby creating a mass transfer of the silicon to the unsaturated areas. This in itself could deplete the contact region. However, it is likely that ohmic contact would be observed. Even if the silicon saturates the aluminum, the electrical conductivity is not degraded extensively. Therefore, the volume ratio may be the cause of depletion, but it is also a suggested mechanism for diffusion.

2.2.5.2 Diffusion Process. It seems evident from the discussion above, that the primary cause for the open resistor circuits was the total transport of the contact silicon into the aluminum during the alloy cycle.

Therefore, it may be stated that due to the non-equilibrium condition which exists during the alloy cycle, the probable mechanism for depleting the silicon entirely from the contact region would be the rapid diffusion of silicon into the aluminum film. The diffusion reaction should be minimized to produce electrically good contacts between the interconnect aluminum film and the poly-crystalline silicon resistors.

2.3 FORMULATION OF SOLUTIONS

To eliminate the contact problem, it was necessary to assume that the failure mode due to diffusion was valid and non-variant. Since the problem was associated with a diffusion process, several methods were proposed to solve the failure. A reduction in the available volume of aluminum into which silicon could diffuse or a method to decrease the amount of silicon diffusing would eliminate the open-circuit failures.

2.3.1 Volume Reduction of Aluminum

The diffusion process which depletes the silicon contact area is dependent on the volume of aluminun available for silicon migration. If the total amount of available aluminum was reduced to its minimum configuration, less diffusion would occur. This postulation may be confirmed by using Fick's first law,

$$J = -D\left(\frac{dc}{dx}\right)$$

where:

J = flux
D = diffusion coefficient
C = concentration
X = distance

The law implies that the quantity of substance diffusing per second through an area of 1 cm^2 is a constant. However, it can be shown that the total quantity diffused during a particular time interval would increase with increasing cross-sectional area. Conversely, a decrease in the total contact area between aluminum and silicon would result in a decrease of silicon depleted at the resistor contact area.

2.3.2 Diffusion Rate

Assuming that the alloy cycle was invariant, the total distance and volume of silicon diffusing would remain constant during a cycle. An alloy cycle has two variables — time and temperature. A reduction in either one would reduce the volume diffused.

2.3.2.1 Temperature Dependency. Reaction rates are temperature-dependent. Assuming a first-order reaction, the reaction would be directly proportional to the temperature. This may readily be confirmed by inspection of the modified Arrhenius Law,

$$k = Ae^{-E/RT}$$

where E is the activation energy.

The adverse or advantageous effects of low-temperature alloying of MOS devices are not fully understood at this time. Therefore, the temperature dependency on the reaction rate should be the last function investigated with respect to eliminating the failure mechanism.

2.3.2.2 Time Dependency. For any diffusion mechanism, a simple control of the total reaction could be accomplished by modulation of the time of reaction. For a first-order reaction, the concentration of the product would be a function of time involved. Therefore, by maintaining a constant temperature, the reaction rate of diffusion would remain a constant, and the total amount diffused would be determined by the total length of time that the reaction was allowed to proceed.

2.3.3 Diffusion Dependency

The open circuits which were observed are caused by the previously described diffusion mechanism. The program to eliminate these failures should investigate a geometrical re-design to reduce the volume ratio aspect and to reduce the time of the alloy cycle to sufficiently impede the reaction prior to total dissolution of silicon.

Section 3
EXPERIMENTATION

3.1 EMPIRICAL INVESTIGATIONS

A test vehicle was designed to provide the necessary information required to fully evaluate the postulates of failure. Primarily, the investigation was used to determine contact geometry dependency and modulated time alloy cycles.

3.1.1 Contact Geometry

The purpose of this experiment was to determine the effect which contact geometry had on the failure mechanism. The initial experiments were conducted by using an invariant alloy cycle. Table I lists the contact geometries investigated.

Table I

Contact Geometry: Si to Al

Oxide Cutout Exposing Silicon (width in μ)	Aluminum Contact Stripe (width in μ)	Remarks
10	50	overlapping Al
10	30	overlapping Al
10	22	overlapping Al
10	10	equivalent Al
30	10	underlapping Al

Several runs were made using the test vehicle. As suspected, the minimum aluminum contact to a large silicon area, i.e., 10 μ Al over 30 μ Si, proved to have the least amount of silicon dissolution. All of the overlapping metal contacts of aluminum indicated that the dissolution was somewhat proportional to the availability of metal. The new accumulator block masks were then designed by using the small metal contact stripe.

3.1.2 Modulation of Alloy Cycles

Upon notice of the decreased failure mechanism utilizing the small metal contact geometry, variations in the alloy time were initiated. The test vehicle also was used initially during these tests. A schedule for alloy time modulation is shown in Table II.

Table II

Alloy Cycle Time Dependency and Failure

Alloy Time at 555°C (minutes)	Dissolution of Silicon
1 to 2	Not observed
2 to 4	Not observed
4 to 6	Primary dissolution
6 to 8	Gross dissolution
> 8	Total dissolution

From the information obtained during these experiments, ohmic contact could be made to all MOS devices and dissolution would not occur if the alloy time were limited to three minutes. It has been observed that there was a two-stepped function. This observation relates to Subsection 2.2.4; investigations of the silicon contact areas, subsequent to metal removal, revealed that maximum solid solubility of silicon into aluminum was attained after two minutes of alloying time. Assuming that the solubility maximum was obtained after two minutes, the addition of one minute of alloy time was required to produce a good ohmic contact to MOS device regions.

3.1.3 Combined Solutions

An alternative was suggested so as to utilize both the alloy cycle perturbations and geometry design. Figure 4 illustrates the proposal. As shown in Fig. 4, the first layer of metal was to be used to contact all points except the resistor contact regions. A second layer of metal was to be delineated, contacting the resistor to the previously alloyed interconnect array. The second layer was to be alloyed at a lower temperature, i.e., 350°C. However, due to the success

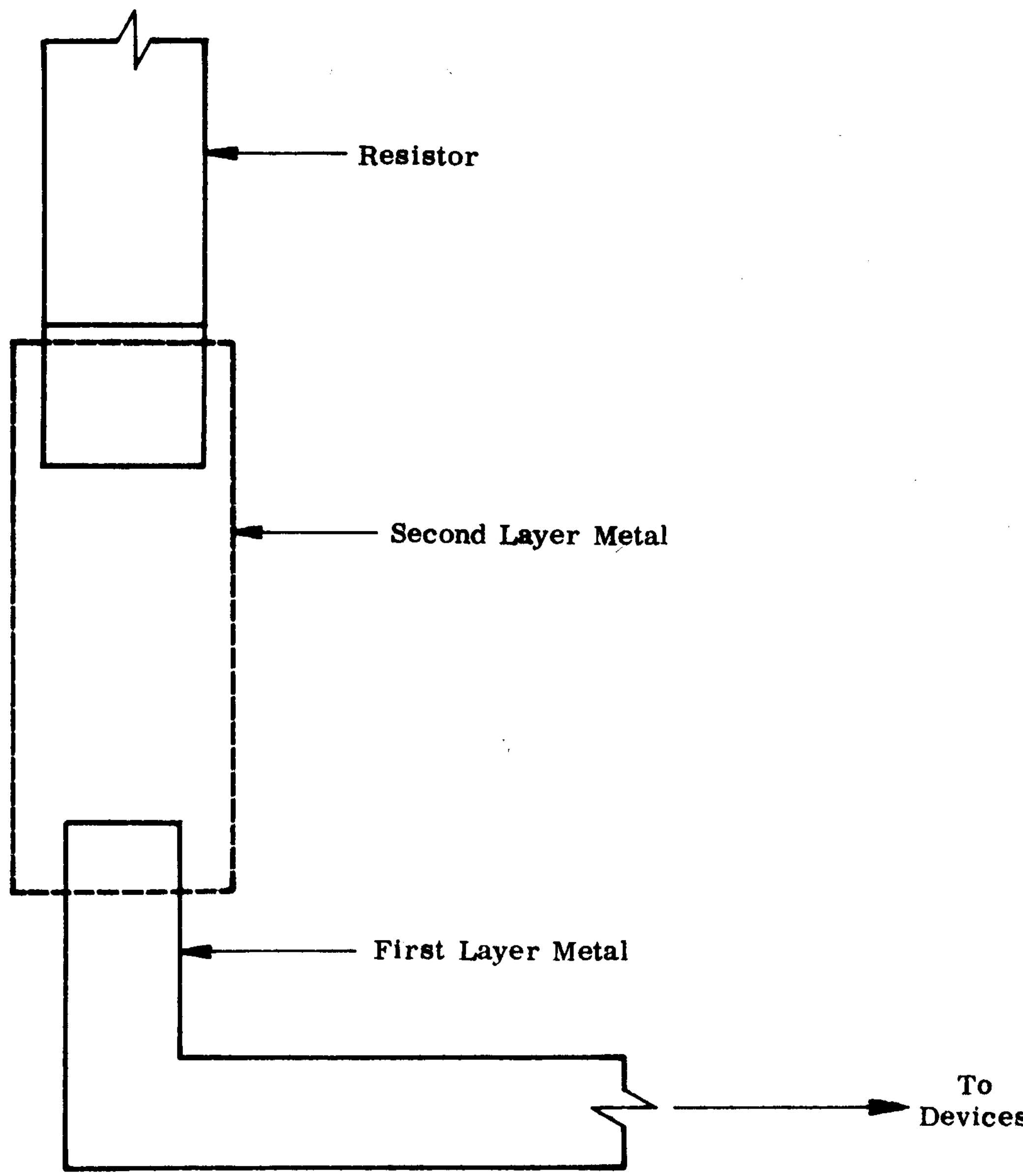


Fig. 4 Double-Masking Low-Temperature Alloy of Second-Layer Metal

of the changes of geometrical design and the limited-time alloy cycle, there has not been a need to use the two-step metallization scheme.

3.1.4 Results of Experiments

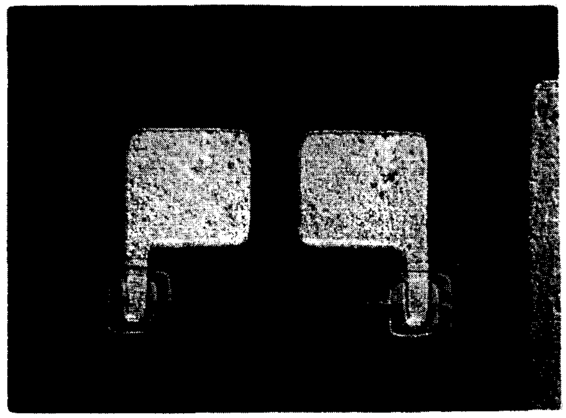
The purpose of the program was to eliminate the contact failure observed electrically as an open circuit. Figure 5 shows a typical resistor contact. These photo-micrographs are taken from an accumulator block which reveals the effects of both the geometry and the modulated time alloy cycle. The precipitates on the contact area probably are due to Si.

The results obtained as shown in Fig. 5 have been reproducible. Work is continuing to provide the required number of accumulator blocks without the contact problem; these will be delivered soon.

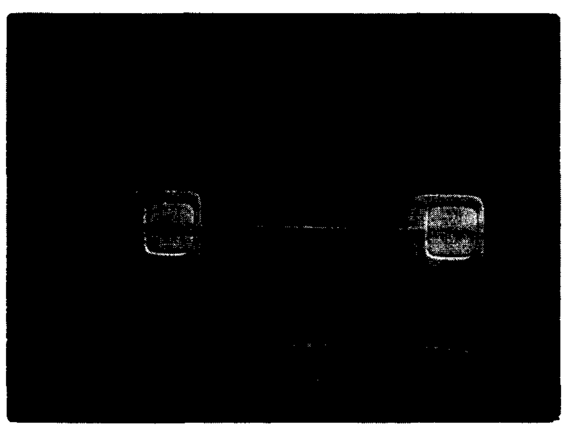
3.2 RELATED OBSERVATIONS

It has been noted that for particular cases the resistor contact area was good, but an open circuit was observed after electrical evaluation. The cause of this type of discontinuity is metal breakage at oxide steps. Primarily, this type of breakage may be solved by the improvement of photo-resist techniques. Considering the hypothetical case depicted in Fig. 6, if the photo-resist had poor adherence to the metal which traverses a large oxide step, undercutting by the delineating etch solution may occur.

It has been suggested that the high stresses concentrated at the knee of the oxide step may be sufficient to separate the metal. This may be true if the metal film is thin. By increasing the thickness of the metal traversing the step, the probability of stress-induced breakage would be reduced.

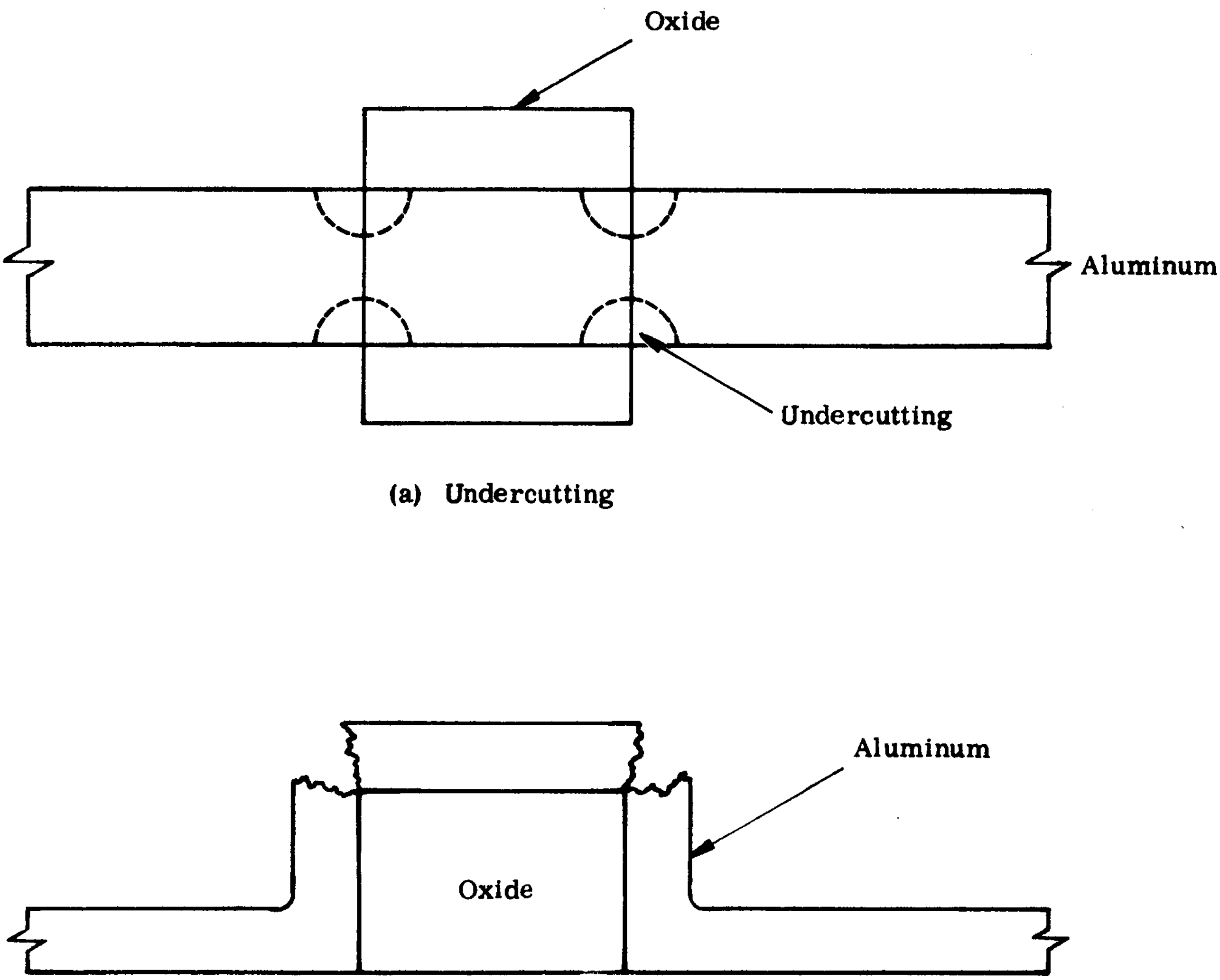


(a) Metal Over Resistor Pads



(b) Metal Removed

Fig. 5 Typical Resistor Contacts



(a) Undercutting

(b) Total Breakage

Fig. 6 Open Circuit Caused by Metal Breakage

3.2.1 Aluminum Deposition Techniques

To decrease the incidence of stress-induced breakage, a thicker deposit is required. On a microscopic scale, the result would appear as shown in Fig. 7.

It is intuitively obvious that the aluminum is decreased in thickness at the point over the oxide step. However, by increasing the total thickness of metal deposited, the ratio of t_1 to t_2 would increase and approach unity. This may be confirmed by assuming that the difference in total oxide height compared to the distance from source to oxide step is infinite, and the impinging aluminum atoms are normal to all surfaces.

Substrate Rotation. It has also been suggested that a rotating substrate holder would ensure that the t_1-to-t_2 ratio approached unity. However, when considering the velocity of an aluminum atom with the velocity obtainable from a rotating substrate holder, the impingement would still appear to be on a stationary surface.

3.2.2 Ratio Increase

Theoretically, it is impossible to have a step which has 90° angles; the optimum is to maintain sloped sides of 45°. This would seem easy to accomplish, since the etching process proceeds at an equal rate both horizontally and vertically. However, undercutting does occur, thereby decreasing the slope to less than 45°. This undercutting then would be beneficial to any metal traversing the slope. Since the slope is slight, the t_1-to-t_2 ratio of metal would increase, since the slope is approximately parallel to all other surfaces.

3.2.3 Solution to Metal Breakage Problem

From the above discussion, improved photo-resist and etching techniques must be maintained prior to and after metal deposition. By increasing the total metal thickness and increasing the t_1-to-t_2 ratio to unity, metal breakage causing open circuits should not be observed.

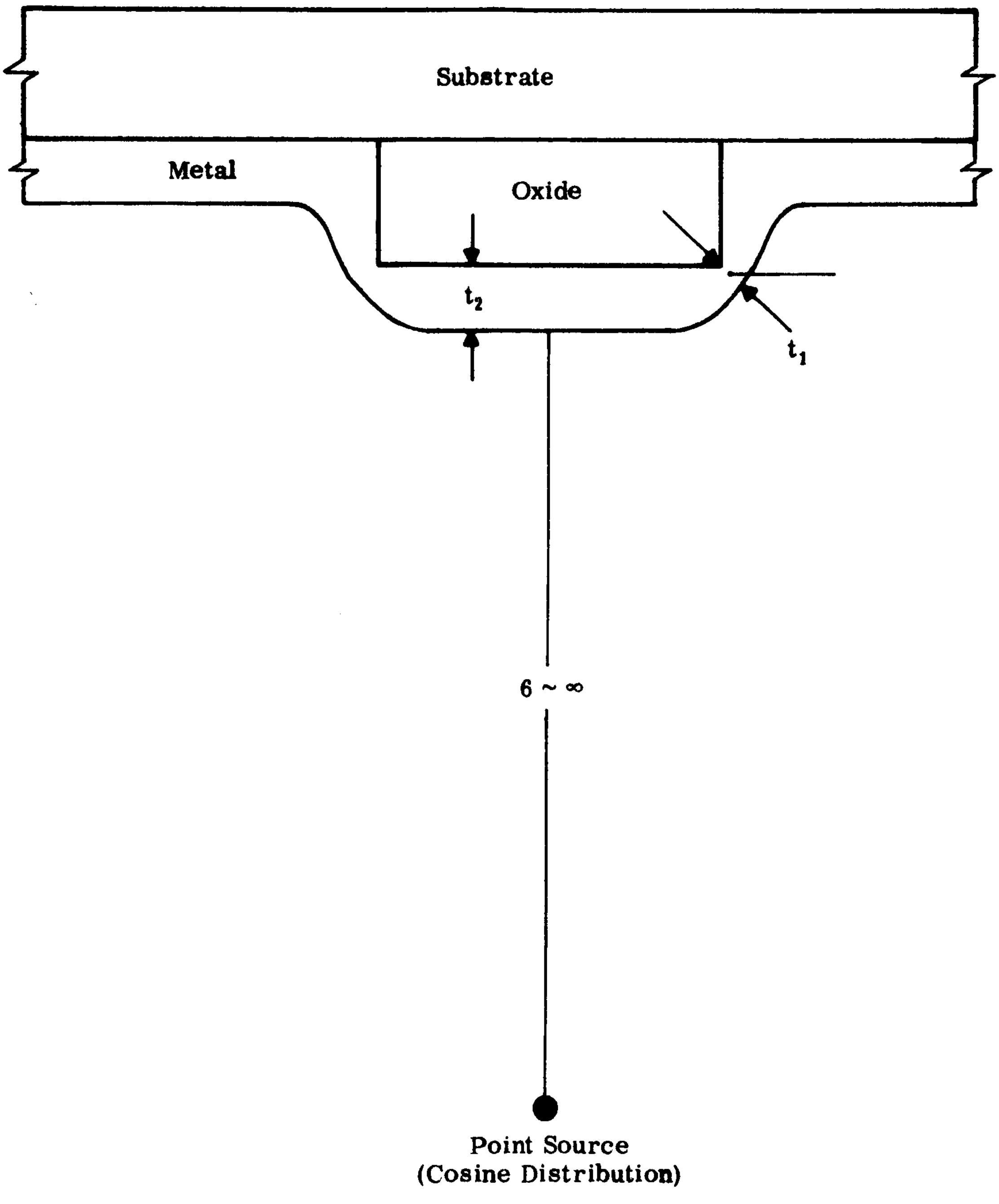


Fig. 7 Relative Increase of Aluminum Thickness

Section 4
CONCLUSION

During the study period, the contact problem associated with aluminum interconnecting films and poly-crystalline silicon, which resulted in an observed open-resistor circuit, was rectified. The failure mode was attributed to the rapid diffusion of silicon away from the contact area. This hypothesis was observed experimentally and solutions were postulated to eliminate the incidence. By optimizing the contacting geometry of aluminum and by adjusting the alloy cycle, the failure mechanism was eliminated. Experimental data on all phases of the investigation will be submitted in a separate report.

Section 5

REFERENCES

1. Rhines, F. N., Phase Diagrams in Metallurgy, McGraw-Hill, New York; 1956
2. Dekker, A. J., Solid State Physics, Prentice-Hall, New Jersey; 1963 Ed.
3. Phillips, A. B., Transistor Engineering, McGraw-Hill, New York; 1962

APPENDIX

A.1 STATUS CHANGE

Due to a change in personnel, Article XIV of NASA contract no. NAS5-9322 should be amended as follows:

R. Gong — Senior Engineer, Project Leader
W. Bailey — Junior Engineer, Process Development
A. Gault — Laboratory Specialist, Processing
C. Swan — Laboratory Specialist, Processing
B. Garcia — Laboratory Specialist, Electrical Testing

A.2 DATA PROCUREMENT

Requirements of items 5, 6, and 7 (Statement of Work) will be delivered with the first shipment of flight quality Philco I and SI blocks.

A.3 SAMPLE CALCULATION

In reference to Subsection 3.2.1 of this report, the most probable velocity of an aluminum molecule would be 2.36×10^4 cm/sec., i.e.,

$$V_p = (2RT/M)^{1/2}$$